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Supporting Information

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Tunable properties of inclusion complexes between amylose and polytetrahydrofuran

Rachmawati Rachmawati, Albert J. J. Woortman, Katja Loos*



Figure S1. Pressure vessel for preparing amylose inclusion complexes.

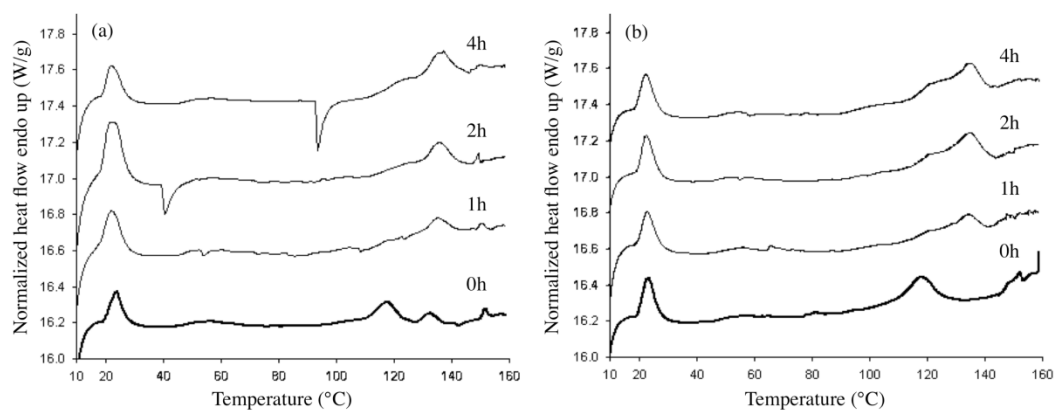


Figure S2. Thermograms of the first heating scan of unwashed inclusion complexes between amylose and PTHF1000 prepared by method OP (a) and method IS (b) from bottom to top: for 0h, 1h, 2h, and 4h complexation time. The endothermic peaks between 20 and 30 °C represent PTHF1000, while the endothermic peaks between 100 and 150 °C represent amylose-PTHF1000 complexes.

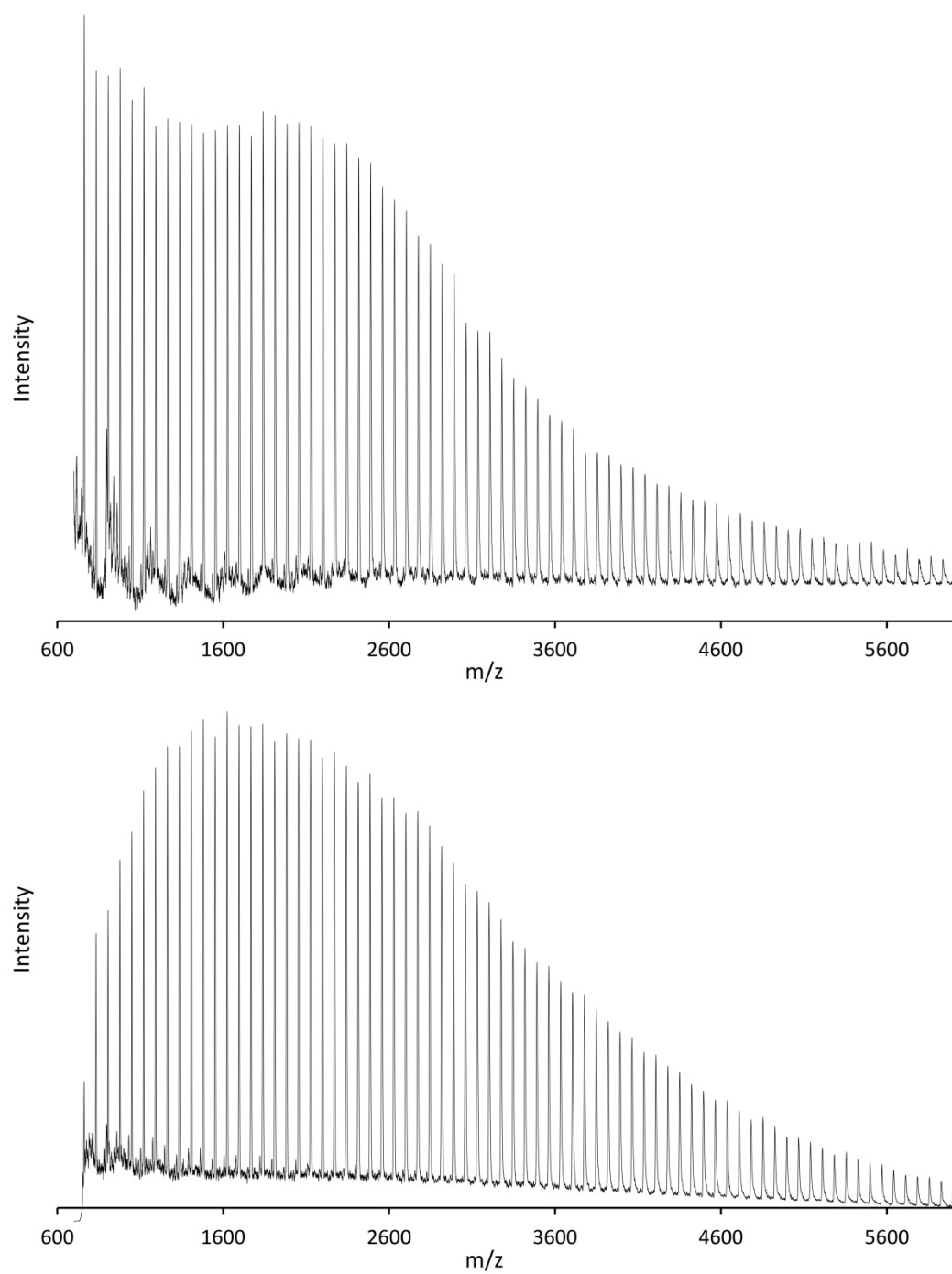


Figure S3. MALDI-ToF-MS spectra of PTHF2000 (top) and sPTHF2000 (bottom).

Table S1. XRD data of amylose-PTHF1000 complexes.

Sample	Main diffractions				Additional diffractions			
	2θ (°)/ d (nm)	Plane (hkl)	2θ (°)/ d (nm)	Plane (hkl)	2θ (°)/ d (nm)	Plane (hkl)	2θ (°)/ d (nm)	Plane (hkl)
Amylose ^{a)}	17.5/0.51		22.9/0.39					
Amylose ^{b)}	17.1/0.52		21.7/0.41					
PTHF1000	19.9/0.45		24.4/0.36					
Inclusion complexes								
0h-unwashed	(13.1)/0.68	200	19.8/0.45	310	(17.5)/0.51	A	(21.0)/0.42	320/450*
0h-W-washed	(13.1)/0.68	200	20.0/0.44	310			(21.0)/0.42	320/450*
1h-unwashed	(13.0)/0.68	200	19.6/0.45	310	16.9/0.52	A	22.1/0.40	002/531*
					(18.5)/0.48	221		
1h-W-washed	12.9/0.69	200	19.7/0.45	310	(17.0)/0.52	201 ^A	21.9/0.41	
					(18.5)/0.48	221		
16h- unwashed	13.1/0.68	200	19.8/0.45	310	16.9/0.52	A	20.9/0.42	
					18.4/0.48	221	22.3/0.40	002/531*
16h-W- washed	13.1/0.68	200	19.8/0.45	310	17.0/0.52	201 ^A	20.3/0.44	
					(18.5)/0.48	221	22.1/0.40	002/531*

^{a)}Untreated; ^{b)}Solubilized and freeze-dried; The d -spacing values are calculated based on Bragg's law for $n = 1$. The hkl values of the diffracting planes are determined based on orthorhombic unit cell of amylose-fatty acids complex^[15], the ones with * sign are based on amylose- n -butanol/ n -pentanol complexes^[16]. The data in brackets are for shoulder-shaped peaks. A denotes amylose.

Table S2. XRD data of amylose inclusion complexes with PTHF2000, sPTHF2000, and PTHF2900.

Inclusion complexes	Main diffractions				Additional diffractions			
	2θ (°)/ d (nm)	Plane (hkl)	2θ (°)/ d (nm)	Plane (hkl)	2θ (°)/ d (nm)	Plane (hkl)	2θ (°)/ d (nm)	Plane (hkl)
Amylose-PTHF2000								
Unwashed	13.1/0.68	200	20.0/0.44	310	(18.5)/0.48	221	22.2/0.40	002
	17.5/0.51	A	24.4/0.36	P	(21.0)/0.42	450*	(28.5)/0.31	411
W-washed	13.2/0.67	111	21.4/0.41	441*	6.9/1.28			
	17.4/0.51	211 ^A	22.7/0.39	311	28.6/0.31	411		
	18.7/0.47	530*	23.7/0.37	222*				
	20.0/0.44	310	24.4/0.36	340 ^P				
Amylose-sPTHF2000								
Unwashed	13.2/0.67	111	19.9/0.45	310	(18.8)/0.47	530*	25.5/0.35	402*
	17.2/0.51	A	24.4/0.36	P	21.3/0.42	450*	26.4/0.34	
W-washed					(21.8)/0.41	441*	27.4/0.33	222
					22.7/0.39	311	28.5/0.31	411
					23.6/0.38	550*		
	13.2/0.67	111	21.4/0.41	441*	7.6/1.16		25.4/0.35	402*
	17.4/0.51	211 ^A	22.6/0.39	311	8.3/1.06		26.5/0.34	422*
	19.9/0.45	310	24.3/0.37	340 ^P	(18.7)/0.47	530*	26.7/0.33	450*
Amylose-PTHF2900					23.4/0.38	550*	27.3/0.33	222
					25.2/0.35	402*	28.5/0.31	411
Unwashed	(13.2)/0.67	111	20.0/0.44	310	(18.2)/0.45		(22.4)/0.40	
	17.3/0.51	A	24.3/0.37	P	19.0/0.47	530*	(23.7)/0.37	222*
W-washed					(21.0)/0.42	450*	25.8/0.34	422*
					(22.1)/0.40		28.5/0.31	411
	(13.3)/0.66	111	23.8/0.37	222*	8.3/1.06		25.4/0.35	402*
	19.9/0.45	310	24.4/0.36	340 ^P	8.9/0.99		26.7/0.33	450*
	21.5/0.41	441*	30.9/0.29	402*	(17.4)/0.51	211 ^A	27.4/0.33	222
					(21.9)/0.41	441*	28.6/0.31	411
(22.4)/0.40								

* hkl values of the diffracting planes are determined based on the orthorhombic unit cell of an amylose-*n*-butanol/*n*-pentanol complexes^[16], while the rest are calculated based on an amylose-fatty acids complex^[15]. The d -spacing values are calculated based on Bragg's law for $n = 1$. The data in brackets are for shoulder-shaped peaks. A and P denote amylose and PTHF.